Study of electronic structure of ytterbium monohydroxide molecule to search for axionlike particles

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Recently the YbOH molecule has been suggested as a candidate to search for the electron electric dipole moment (eEDM) which violates spatial parity (P) and time-reversal (T) symmetries [Phys. Rev. Lett. **119**, 133002 (2017)]. In the present paper we show that the same system can be used to measure coupling constants of the interaction of electrons and nucleus with axionlike particles. The electron-nucleus interaction produced by the axion exchange induces T,P-violating a EDM of the whole molecular system. We express the corresponding T,P-violating energy shift produced by this effect in terms of the axion mass and product of the axion-nucleus and axion-electron coupling constants.

I. INTRODUCTION

Verification of the Standard Model (SM) and its extensions is of key importance for modern theoretical physics and cosmology [1]. Despite numerous experimental confirmations of the SM, several observed phenomena cannot be explained in its frames. Among them are the strong CP-problem of quantum chromodynamics (QCD), the unknown nature of dark matter and dark energy and the problem of the baryogenesis [2].

A possible solution of the strong CP-problem was suggested by Peccei and Quinn [3] via modification of the QCD Lagrangian. Weinberg and Wilczek also independently noticed that the spontaneous Peccei-Quinn $U_{PQ}(1)$ symmetry violation demands the existence of the pseudoscalar Goldstone boson, afterwards called the axion [4, 5]. Later it was realized that the axion is a suitable candidate to be the dark matter component [6–8]. Therefore, it also solves another aforementioned problem of the SM. In the QCD axion case there are relations connecting axion mass and axion-fermion interaction strength. In a more general case of axionlike particles no such connection is assumed. Numerous experimental investigations led to strong constraints on the axionlike particle properties [9–11] (see also Fig. 2 in Ref. [12]). For brevity axionlike particles are often called axions, without assuming the QCD axion properties.

It is known that the search for T,P-violating effects such as the electron electric dipole moment (eEDM) in the low-energy regime can be successfully performed with paramagnetic heavy atoms and small molecules containing such atoms [1, 13, 14]. One of the benefits of such molecules is the existence of closely lying opposite parity levels enhancing eEDM effect [15]. For instance, the strongest current constraints on the eEDM value d_e is obtained in an experiment using a thorium monoxide molecular beam [16]. Other molecular experiments [17, 18] also surpass sensitivity of atomic EDM experiments [19]. The axion-induced T,P-violating effects can also be measured in these molecular experiments [12, 20].

It was recently suggested to perform experiments to search for the electron electric dipole moment using linear triatomic molecules containing heavy atoms. These molecules have a very small energy gap between opposite parity levels due to l-doubling effect [21–23]. This feature makes it possible to polarize them by relatively weak electric field. Besides, these molecules can be cooled and slowed by the laser-cooling technique to extremely low temperatures [24]. This is the way to increase the coherence time and, thus, to improve the sensitivity of the experiment as the uncertainty of the measured energy characteristic is inversely proportional to the coherence time. For this reason, the YbOH molecule has been intensively considered for the T,P-violating effect search by several theoretical groups [25–28].

In Ref. [12] the first estimations of the axion-induced interactions in a number of diatomic molecules have been performed. These estimations have been based on atomic calculations and scaling. In the present paper we introduce an explicit molecular approach to study the axion-mediated T,P-violating interaction based on the relativistic Fock-space coupled cluster theory. The dependence of the corresponding energy shift on the axionlike particle mass is considered in the ytterbium monohydroxide (YbOH) molecule. It is shown that the expected sensitivity [22] of the experiment on this molecule will enable to set limits on the axionlike particle coupling constants surpassing current limits by several orders of magnitude.

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II. THEORY

The coupling of an axionlike particle a with the SM fermions ψ can be written in the following form:

$$\mathcal{L}_{\text{int}} = a \sum_{\psi} \bar{\psi} \left(g_{\psi}^s + i g_{\psi}^p \gamma_5 \right) \psi. \qquad (1)$$

The coupling constants g_{ψ}^s and g_{ψ}^p characterize the scalar and pseudoscalar interactions in the Lagrangian (1). This mixed scalar and pseudoscalar interaction leads to T,P-violating effects.

The electron pseudoscalar and nucleon scalar interactions in Eq. (1) with the intermediate boson a of the mass m_a lead to the T,P-violating Yukawa-type interaction potential [12]:

$$V_{\text{eN}}(\boldsymbol{r}) = +i \frac{g_N^s g_e^p}{4\pi} \frac{e^{-m_a|\boldsymbol{r}-\boldsymbol{R}|}}{|\boldsymbol{r}-\boldsymbol{R}|} \gamma^0 \gamma_5. \qquad (2)$$

Here $\boldsymbol{r}$ and $\boldsymbol{R}$ are positions of the electron and nucleus under consideration, respectively; γ–matrices are Dirac matrices defined according to [29] and refer to the electron; g_N^s and g_e^p are the coupling constants of the axionlike particle with the nucleus and the electron, respectively. This interaction has a similar form as the T,P-violating contact nucleus-electron scalar-pseudoscalar interaction [13]:

$$H_{T,P} = +i \frac{G_F}{\sqrt{2}} Z k_{T,P} n(\mathbf{r}) \gamma^0 \gamma_5, \qquad (3)$$

where G_F is the Fermi-coupling constant, Z is the nuclear charge, $k_{T,P}$ is the coupling constant and $n(\mathbf{r})$ is the nuclear density normalized to unity. It should be noted that this form of the interaction (2) corresponds to the interaction of axion with electron spin. Interaction of axion with nucleon spin is considered in Ref. [30].

Inclusion of the interaction (2) into the electronic Hamiltonian leads to T,P-violating energy shifts of electronic states in a manner analogous the shifts created by the nucleus-electron scalar-pseudoscalar interaction. This shift is proportional to $g_N^s g_e^p$ and can be characterised by the molecular constant $W_{\text{ax}}^{(\text{eN})}$ which depends on the axionlike particle mass m_a:

$$W_{\text{ax}}^{(\text{eN})}(m_a) = \frac{1}{g_N^s g_e^p} \langle \Psi | \sum_{i=1}^{N} V_{\text{eN}}(\boldsymbol{r}_i) | \Psi \rangle. \qquad (4)$$

Here index i runs over all electrons in the molecule, and Ψ is the electronic wavefunction. The characteristic T,P-violating energy shift of the electronic level can be expressed as [31]:

$$\delta E = g_N^s g_e^p \cdot W_{\text{ax}}^{(\text{eN})}(m_a). \qquad (5)$$

The value of $W_{\text{ax}}^{(\text{eN})}$ is required for interpretation of the experimental data in terms of the product of interaction constants. This molecular constant is the analog of the effective electric field and the molecular constant $W_{T,P}$ that characterizes molecular parameter of the scalar-pseudoscalar nucleus-electron interaction in the electron electric dipole moment search area (see e.g. [27, 28, 32–37]). Note, however, that in the present case $W_{\text{ax}}^{(\text{eN})}$ depends on the axion mass. The typical radius of the interaction Eq. (2) can be estimated as $R_{\text{Yu}}(m_a) \simeq \frac{3730}{(m_a/\text{eV})} a_B$, where a_B is the Bohr radius. As it is shown below, in the limiting case of large R_{Yu} the $W_{\text{ax}}^{(\text{eN})}$ constant is almost independent on m_a and in the opposite limiting case of high-mass axionlike particles the factorization of the $W_{\text{ax}}^{(\text{eN})}$ is possible.

In the present paper we calculate molecular constant $W_{\text{ax}}^{(\text{eN})}(m_a)$ for the YbOH molecule over a wide range of m_a values. The molecule is considered in its ground $^2\Sigma_{1/2}$ electronic state.

The equilibrium geometry parameters of the molecule are $R(\text{Yb-O}) = 2.037$Å and $R(\text{O-H}) = 0.951$Å, the molecule is linear [38, 39].

In the electronic structure calculations we have used one-particle molecular bispinors obtained within the Dirac-Hartree-Fock approach using the Gaussian-type basis sets. In order to estimate the basis set size dependence of the $W_{\text{ax}}^{(\text{eN})}$ parameter, the calculations were performed within four basis sets, which are described in Table I. These basis sets are ordered by its quality, i.e. the basD is the best considered basis set. For Yb we have used Dyall's family of all-electron uncontracted basis sets.

TABLE I. Notation and composition of the basis sets used.

Basis set notation	basis on Yb [40]	basis on O and H [41–43]*
basA	AE2Z [24s,19p,13d,8f,2g]	aug-cc-pVDZ-DK [10s,5p,2d] and [5s,2p]
basB	AE3Z [30s,24p,16d,11f,4g,2h]	aug-cc-pVDZ-DK [10s,5p,2d] and [5s,2p]
basC	AE3Z [30s,24p,16d,11f,4g,2h]	aug-cc-pVTZ-DK [11s,6p,3d,2f] and [6s,3p,2d]
basD	AE4Z [35s,30p,19d,14f,8g,5h,2i]	aug-cc-pVTZ-DK [11s,6p,3d,2f] and [6s,3p,2d]

*The basis sets on O and H were uncontracted.

Electronic correlation effects have been taken into account using the relativistic Fock-space coupled cluster approach with single and double cluster amplitudes (FS-CCSD) [44] within the finite field approach. Fock-space sector (0,0) corresponds to the YbOH$^+$ cation in its ground electronic state, and open-shell electronic calculations were performed in sector (0,1). All electrons of YbOH have been included in correlation calculations. In Refs. [37, 45] it has been shown that high energy cut-off is important to ensure including functions that describe spin-polarization and correlation effects for core

electrons. In the present paper all virtual orbitals have been included in correlation treatment. The effect of the Gaunt interaction of the electrons was estimated within the Dirac-Hartree-Fock-Gaunt approach using the basD basis set. Its relative contribution reaches the maximal value of -2.2% for $m_a = 10^4$ eV and does not exceed 1% by absolute value for other presented m_a. It was shown in [46], that electronic correlation can affect the Gaunt contribution to the properties of triatomic molecules, but the absolute value contribution is not significant. We do not include the Gaunt contribution to the values in Table III.

Both the Dirac-Hartree-Fock and the Fock-space calculations were performed using the local version of the DIRAC15 code [47]. The code to calculate matrix elements of the electron-nucleus interaction Eq. (2) was developed in the present paper.

III. RESULTS AND DISCUSSION

Tables II and III give the calculated dependence of the $W_{\rm ax}^{\rm (eN)}$ value on the mass of the axionlike particle m_a using different basis sets and methods. The final values are given in the last column of Table III. The uncertainty of the final values arises mainly from higher-order correlations and can be estimated to be less than 10% [25].

TABLE II. The values of the $W_{\rm ax}^{\rm (eN)}$ constant for the ground electronic state of YbOH (in units of $m_e c/\hbar$) for various m_a using the Dirac-Hartree-Fock method and different basis sets.

m_a, eV	basA	basB	basC	basD
10	$+1.12 \cdot 10^{-5}$	$+1.11 \cdot 10^{-5}$	$+1.11 \cdot 10^{-5}$	$+1.11 \cdot 10^{-5}$
10^2	$+1.11 \cdot 10^{-5}$	$+1.11 \cdot 10^{-5}$	$+1.11 \cdot 10^{-5}$	$+1.11 \cdot 10^{-5}$
10^3	$+9.23 \cdot 10^{-6}$	$+9.17 \cdot 10^{-6}$	$+9.17 \cdot 10^{-6}$	$+9.15 \cdot 10^{-6}$
10^4	$+1.35 \cdot 10^{-6}$	$+1.34 \cdot 10^{-6}$	$+1.33 \cdot 10^{-6}$	$+1.33 \cdot 10^{-6}$
10^5	$-5.06 \cdot 10^{-6}$	$-5.02 \cdot 10^{-6}$	$-5.02 \cdot 10^{-6}$	$-5.01 \cdot 10^{-6}$
10^6	$-3.79 \cdot 10^{-6}$	$-3.76 \cdot 10^{-6}$	$-3.76 \cdot 10^{-6}$	$-3.75 \cdot 10^{-6}$
10^7	$-1.60 \cdot 10^{-7}$	$-1.60 \cdot 10^{-7}$	$-1.60 \cdot 10^{-7}$	$-1.59 \cdot 10^{-7}$
10^8	$-2.67 \cdot 10^{-9}$	$-2.85 \cdot 10^{-9}$	$-2.85 \cdot 10^{-9}$	$-2.88 \cdot 10^{-9}$
10^9	$-2.82 \cdot 10^{-11}$	$-3.09 \cdot 10^{-11}$	$-3.09 \cdot 10^{-11}$	$-3.17 \cdot 10^{-11}$
10^{10}	$-2.83 \cdot 10^{-13}$	$-3.10 \cdot 10^{-13}$	$-3.10 \cdot 10^{-13}$	$-3.17 \cdot 10^{-13}$

As one can see from Tables II and III, results for low-mass axionlike particles are weakly dependent on the basis set size. However, according to our findings, basis functions with small radii should be included in the basis set to describe correctly the electronic wavefunction asymptotic in the vicinity of a heavy nucleus in the heavy axion case. It can be seen from comparison of Tables II and III that the role of correlation effects increases for high m_a values. Note that in the region from 10^4 eV to 10^5 eV the $W_{\rm ax}^{\rm (eN)}$ constant changes its sign. This can be explained by the fact that the effects for low-mass and

TABLE III. The values of the $W_{\rm ax}^{\rm (eN)}$ constant for the ground electronic state of YbOH (in units of $m_e c/\hbar$) for various m_a using the relativistic FS-CCSD approach and different basis sets.

m_a, eV	basA	basB	basC	basD (Final)
10	$+1.28 \cdot 10^{-5}$	$+1.31 \cdot 10^{-5}$	$+1.31 \cdot 10^{-5}$	$+1.32 \cdot 10^{-5}$
10^2	$+1.27 \cdot 10^{-5}$	$+1.31 \cdot 10^{-5}$	$+1.30 \cdot 10^{-5}$	$+1.32 \cdot 10^{-5}$
10^3	$+1.09 \cdot 10^{-5}$	$+1.13 \cdot 10^{-5}$	$+1.12 \cdot 10^{-5}$	$+1.14 \cdot 10^{-5}$
10^4	$+1.38 \cdot 10^{-6}$	$+1.51 \cdot 10^{-6}$	$+1.51 \cdot 10^{-6}$	$+1.57 \cdot 10^{-6}$
10^5	$-7.02 \cdot 10^{-6}$	$-7.22 \cdot 10^{-6}$	$-7.21 \cdot 10^{-6}$	$-7.30 \cdot 10^{-6}$
10^6	$-5.20 \cdot 10^{-6}$	$-5.33 \cdot 10^{-6}$	$-5.32 \cdot 10^{-6}$	$-5.37 \cdot 10^{-6}$
10^7	$-2.20 \cdot 10^{-7}$	$-2.26 \cdot 10^{-7}$	$-2.26 \cdot 10^{-7}$	$-2.28 \cdot 10^{-7}$
10^8	$-3.66 \cdot 10^{-9}$	$-4.03 \cdot 10^{-9}$	$-4.03 \cdot 10^{-9}$	$-4.11 \cdot 10^{-9}$
10^9	$-3.87 \cdot 10^{-11}$	$-4.38 \cdot 10^{-11}$	$-4.37 \cdot 10^{-11}$	$-4.52 \cdot 10^{-11}$
10^{10}	$-3.88 \cdot 10^{-13}$	$-4.39 \cdot 10^{-13}$	$-4.38 \cdot 10^{-13}$	$-4.53 \cdot 10^{-13}$

high-mass axions arise from different distances [12]. Below we discuss separately the low- and the high-mass axion cases. In the latter case the potential (2) is spatially localized in the vicinity of the nucleus and in this case the $W_{\rm ax}^{\rm (eN)}$ parameter belongs to the class of the "atom in a compound" (AiC) characteristics [48–50]. This means that it should have similar correlation trends to other characteristics such as the effective electric field acting on the electron electric dipole moment, etc.

Low-mass limit. As one should expect from the potential form (2) and as it can be seen from Table III, for $m_a \ll 10^3$ eV the $W_{\rm ax}^{\rm (eN)}$ parameter is almost independent on m_a. Thus, for the low-mass axion case we can explicitly obtain the link between the $g_N^s g_e^p$ product and the energy shift δE defined by Eq. (5) employing the electronic structure calculation. The mass of the axionlike particle becomes unimportant here. The current limitation for these interaction constants product $|g_N^s g_e^p|/(\hbar c) \lesssim 10^{-19}$ [12] can be obtained from the interpretation of the second generation of the ThO experiment [51]. Note, that this constraint is the strongest for $m_a \gtrsim 10^{-2}$ eV (see Fig. 2 in Ref. [12]). The corresponding energy shift in the YbOH molecule would be $\delta E \simeq 160$ μHz. This value has the same order of magnitude as the sensitivity to T,P-violating effects already achieved in the ThO experiment [16]. In Ref. [22] it was suggested that using the YbOH molecule the sensitivity to the electron EDM could be increased by up to 4 orders of magnitude above the that obtained in [52] (and, consequently, 3 orders with respect to Ref [16]). Therefore, the expected sensitivity of the YbOH experiment will ultimately be enough to set orders of magnitude stronger limitations on $|g_N^s g_e^p|$.

High-mass limit. For axions with mass $m_a \gg 10^6$ eV the approximate dependence is $W_{\rm ax}^{\rm (eN)} \simeq \widetilde{W} \cdot m_a^{-2}$, where the $\widetilde{W}$ value does not depend on m_a. In this case, the

measured energy shift can be parameterized as

$$\delta E \approx \frac{g_N^s g_e^p}{m_a^2} \widetilde{W},$$ (6)

and the constraint for the combination $g_N^s g_e^p / m_a^2$ can be derived from the experimental data. The constraint $|g_N^s g_e^p| / (\hbar c m_a^2) \lesssim 10^{-14} \text{ GeV}^{-2}$ can be obtained from the interpretation of the experiment with the ThO molecule [12, 16]. The energy shift in the YbOH molecule corresponding to this constraint would be ~ 60 μHz. As it has been noted above, the ultimate sensitivity of the YbOH experiment is several orders higher. Thus, in the high-mass limit it also will be possible to obtain new constraints.

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